2-Ethoxyethyl acetate 111-15-9 | DTXSID9021928

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Model	Data	

Weighted KNN model

5-fold CV (75%)		Training (75	Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.85	0.69	0.86	0.67	0.86	0.78	

Model Results

Predicted value: 5.94e-01

Global applicability domain: Inside

Local applicability domain index: 6.27e-01

Confidence level: 8.26e-01

Nearest Neighbors from the Training Set

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1-Methoxy-2-propyl acetate

Measured: 0.56 Predicted: 4.87e-01

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Diethyl oxalate Measured: 0.56 Predicted: 4.01e-01

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Acetic acid, difluoro-, ethyl ester

Measured: 0.87 Predicted: 8.28e-01

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2,2-Dimethyl-1,3-dioxolane

Measured: 0.46 Predicted: 5.11e-01

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2-Methoxyethyl acrylate

Measured: 0.56 Predicted: 4.66e-01